

Semiclassical methods for multi-dimensional systems bounded by finite potentials

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(Dated: February 2, 2008)

This work studies the semiclassical methods in multi-dimensional quantum systems bounded by finite potentials. By replacing the Maslov index by the scattering phase, the modified transfer operator method gives rather accurate corrections to the quantum energies of the circular and square potential pots of finite heights. The result justifies the proposed scattering phase correction which paves the way for correcting other semiclassical methods based on Green functions, like Gutzwiller trace formula, dynamical zeta functions, and Landauer-Büttiker formula.

PACS numbers: 03.65.Sq, 05.45.Mt, 03.65.Ge

Semiclassical approaches are techniques to study quantum systems in classical limit [1]. In these approaches, physical quantities are expressed by the Green function of the system and replaced by its underlying classical trajectories under stationary phase approximation. Well known examples range over Gutzwiller trace formula, dynamical zeta function, and transfer operators, which are aimed at determining the quantized energies of closed systems [1]. For open systems, the most prominent example might be the Landauer-Büttiker formula for charge current transport through open quantum dots [2]. Recently semiclassical approaches also have been used to study spin current transport [3] and spin dynamics, which clarifies the suppression of D'yakonov-Perel' spin relaxation in mesoscopic quantum dots [4]. All these approaches can relate quantum problems to the ergodicity property of their corresponding classical dynamics and gives more transparent pictures to complex phenomena, including the signatures of quantum chaos [1].

Besides this conceptual contribution, some semiclassical methods provide efficient numerical techniques for less time-consuming calculations. Their results are especially accurate in mesoscopic systems in which the de Broglie wavelength of the Fermi electrons is much shorter the sample size. The devices in this scale are often fabricated by lithography or controlled by confining potentials. A convenient theoretical approach to study these quantum systems is assuming them to be bounded by infinite potential. This largely simplifies the formulism of the semiclassical methods, since the quantum particle has the same phase change for arbitrary particle energy after it is reflected by this potential. This phase change is carried in the well known Maslov index. However, for real systems beyond this assumption, the accuracy of the conventional semiclassical methods using Maslov index become out of control. The usual way is going back to solve the Schrödinger equation with a boundary combined with Dirichlet and von Neuman conditions. But one could ask whether the conventional semiclassical methods still work after taking certain effective correction.

A natural candidate for this correction is an effective phase change in the wave function after it is bounced back by the potential. This phase can be understood as the dwell time of the quantum particle penetrating into and staying inside the potential barrier. Indeed, in the one-dimensional (1D) potential well, it has been shown that replacing the Maslov index in the Green function by a scattering phase, this function gives an exact quantization rule identical with the Wentzel-Kramers-Brillouin (WKB) method [7]. This relation stirs up the motivation how to extend this result to multi-dimensional systems. The current paper demonstrates this extension in the example of Bogomolny's transfer operator (BTO) method [9] and tested it in a circular billiard and a square billiard bounded by potential pots of finite height. The calculated energies are surprisingly accurate, which justifies the suggested scattering phase correction for multi-dimensional systems. Although the result is presented in the BTO method, it should be valid for all semiclassical methods as long as they are based on the Green function.

The WKB method might be the simplest semiclassical method. For a particle of mass m and energy E bounded by an 1D potential $V(x)$, the solution of its Schrödinger equation can be approximated by the WBK wave function [5],

$$\psi(x) = \frac{1}{\sqrt{p(x)}} \exp \left[\pm \int_{x_i}^x p(x') dx' \right], \quad (1)$$

with $p(x) = \sqrt{2m[E - V(x)]}$, if the de Broglie wavelength $\lambda(x) = 2\pi\hbar/p(x)$ varies slowly compared to the potential. This requirement is usually violated at the classical turning point x_0 , where the momentum changes sign. At that point one has $E = V(x_0)$ which gives rise to a vanishing $p(x_0)$ and a singular function $\psi(x)$. If the potential varies slowly around x_0 , the exponentially decreasing real wave function outside this point should be associated with the oscillating wave function inside this point. This enforces the incident wave function to take a *scattering phase* after reflection. This phase is equal to $\pi/2$ in the semiclassical (short wave) limit [5]. If the

particle is reflected back and forth between two turning points x_1 and x_2 on two potential barriers, the particle should take two scattering phases $\phi_1 = \phi_2 = \pi/2$ during one period of motion. The total phase then equals $2n\pi$ with an integer n , which leads to the WKB quantization condition [5]

$$\frac{1}{\hbar} \oint p(x) dx = \frac{2}{\hbar} \int_{x_1}^{x_2} p(x) dx = 2\pi \left(n + \frac{\mu}{4} \right), \quad (2)$$

where the Maslov index $\mu = 2$ corresponds to the two reflections during one period of particle motion.

If the potential does not vary sufficiently slowly at the turning points, for example the step function barrier, the phase change $\pi/2$ is no longer a good approximation. A general scattering phase should be determined quantum-mechanically [6],

$$\frac{1}{\hbar} \oint p(x) dx = 2n\pi + \phi_1(E) + \phi_2(E), \quad (3)$$

where the phase changes $\phi_1(E)$ and $\phi_2(E)$ at the turning points x_1 respectively x_2 become a function of E . As an example, let this particle move in an 1D finite square well with $V(x) = 0$ for $0 < x < L$ and V_0 otherwise, where L is the well width and $V_0 > 0$ is the potential height. Solving the Schrödinger equation with the continuous boundary condition, the scattering phase can be calculated,

$$\phi_s(E) = \cos^{-1} \left[2 \left(\frac{E}{V_0} \right) - 1 \right]. \quad (4)$$

Substituting Eq. (4) into $\phi_1(E)$ and $\phi_2(E)$ in Eq. (3), one obtains an exact quantization rule for the 1D finite square well.

For general k -dimensional systems with $k \geq 2$, many quantization rules have been derived to extend the WKB method, including Gutzwiller trace formula, dynamical zeta function, and transfer operators [1]. All of them are based on the semiclassical Green function

$$G(\mathbf{r}, \mathbf{r}'; E) = \frac{1}{(2\pi i \hbar)^{k/2}} \sum_{\gamma} \sqrt{\left| \det \frac{\partial S_{\text{cl}}(\mathbf{r}, \mathbf{r}'; E)}{\partial \mathbf{r} \partial \mathbf{r}'} \right|} \times \exp \left[\frac{i}{\hbar} S_{\text{cl}}(\mathbf{r}, \mathbf{r}'; E) - i\mu \frac{\pi}{2} \right], \quad (5)$$

which is a sum over all classical trajectories γ starting from \mathbf{r}' and ending at \mathbf{r} [1, 8]. The function $S_{\text{cl}}(\mathbf{r}, \mathbf{r}'; E)$ therein is the action of the particle from \mathbf{r}' to \mathbf{r} along γ . The Maslov index μ stands for the total number of the turning points between \mathbf{r}' and \mathbf{r} along γ . For 1D finite square well, the quantization rule derived from Eq. (5) with the replacement $\mu \frac{\pi}{2}$ by ϕ_s in Eq. (4) is identical with the quantization rule of Eq. (3) with the same phase correction ϕ_s [7].

For multi-dimensional systems, intuitively, the magnitude of the scattering phase should depend on the incident angle of the particle wave. Naively one could suggest

the phase ϕ_s in Eq. (4) to be only related to the perpendicular component of the incident wave with respect to the boundary. Figure 1(a) shows an example of a 2D step potential $V_c(x, y) = V_0 \Theta(x)$ with the potential high $V_0 > 0$ for $x \geq 0$ and 0 for $x < 0$, where $\Theta(x)$ is the Heviside function. The momentum p_x perpendicular to the boundary has energy $E_p = p_x^2/2m$, which will replace the total energy E in Eq. (4) for multi-dimensional systems. This phase is a value between 0 and π , depending on the ratio E_p/V_0 , as shown in Fig. 1(b). If the potential barrier is high, that is $E_p/V_0 \ll 1$, the scattering phase will approach π , which is the same as the infinitely high potential barrier.

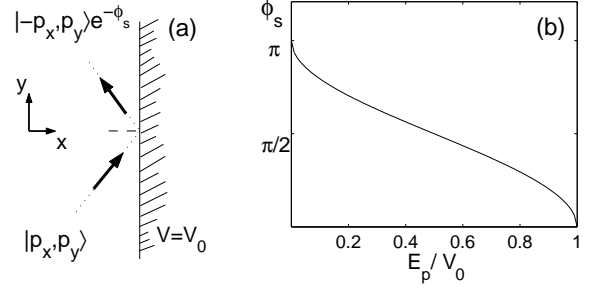


FIG. 1: (a) The incident state $|p_x, p_y\rangle$ and the reflected state $|-p_x, p_y\rangle e^{-i\phi_s}$ on the confining potential V_0 . (b) The scattering phase ϕ_s of the reflected state is a function of E_p/V_0 .

Next, the scattering phase for the perpendicular wave component discussed above will be merged into BTO method. Let us consider again the particle of mass m and energy E moving in a k -dimensional system. Select a Poincaré section (PS) Σ in the configuration space of this system, such that almost all classical trajectories pass this section [10]. The original transfer operator $\mathcal{T}(E)$ is defined as the integral operator [9]

$$\mathcal{T}(E)\psi(q) = \int_{\Sigma} T(q, q'; E) \psi(q') dq', \quad (6)$$

acting on some function $\psi(q')$ on Σ . The integral kernel,

$$T(q, q'; E) = \sum_{\gamma} \frac{1}{(2\pi i \hbar)^{(k-1)/2}} \sqrt{\left| \det \frac{\partial S_{\text{cl}}(q, q'; E)}{\partial q \partial q'} \right|} \times \exp \left[\frac{i}{\hbar} S_{\text{cl}}(q, q'; E) - i\nu \frac{\pi}{2} \right], \quad (7)$$

is defined as the sum over all possible classical trajectories γ 's from the initial point $q' \in \Sigma$ to the final point $q \in \Sigma$. The action $S_{\text{cl}}(q, q'; E)$ is the same as before in Eq. (5). The Maslov index ν counts the number of the crossing points of γ through Σ from the same side of Σ . According to the BTO method, the zeros of the Fredholm determinant $|\det(1 - \mathcal{T}(E))|$ of the transfer operator $\mathcal{T}(E)$ are the energy eigenvalues of the quantum system.

The kernel in Eq. (7) is derived from the semiclassical Green function in Eq. (5), which can be divided into two parts, $G(q, q'; E) = G^{\text{osc}}(q, q'; E) - G_0(q, q'; E)$, where $G^{\text{osc}}(q, q'; E)$ is the contribution from long trajectories and $G_0(q, q'; E)$ is the contribution from short trajectories. After coordinate deduction from k -dimensional space to $(k-1)$ -dimensional space on Σ [9], the quantization condition $|\det(G(q, q'; E))| = 0$ can be expressed as $|\det(1 - \mathcal{T}(E))| = 0$, where the identity operator comes from G_0 and the operator $\mathcal{T}(E)$ originates from G^{osc} . The entire derivation holds the same when the phase in $G(q, q'; E)$ is modified. The transfer operator $\mathcal{T}_m(E)$ modified with the scattering phase for perpendicular wave component then has the kernel

$$T_m(q, q'; E) = \sum_{\gamma} \frac{1}{(2\pi i \hbar)^{(k-1)/2}} \sqrt{\left| \det \frac{\partial S_{\text{cl}}(q, q'; E)}{\partial q \partial q'} \right|} \times \exp \left[\frac{i}{\hbar} S_{\text{cl}}(q, q'; E) - i \phi_s(E_p) \right]. \quad (8)$$

The efficiency of this modified operator will be tested in the following two 2D integrable systems.

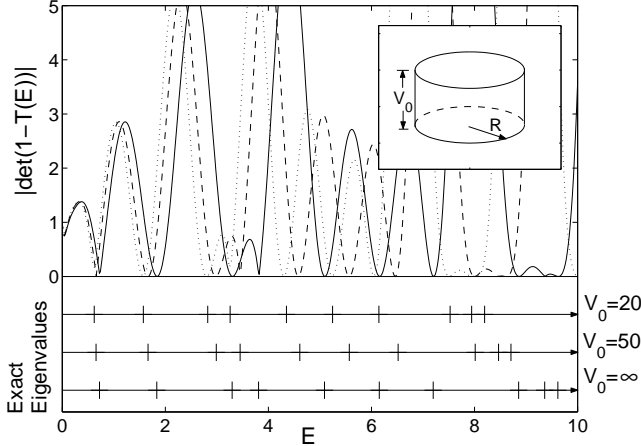


FIG. 2: The upper part shows the Fredholm determinant $|\det(1 - \mathcal{T}_m(E))|$ of the modified transfer operator $\mathcal{T}_m(E)$ for the potential pot in the inset for $V_0 = 20, 50$, and ∞ with $R = 2$. The points on the three bottom lines depict the exact quantum energies for $V_0 = 20, 50$, and ∞ with $R = 2$.

The first system is a 2D circular quantum dot bounded by a finite potential, as shown in the inset of Fig. 2. The potential pot has radius R and height V_0 , that is $V(r) = V_0$ for $r \geq R$ and $V(r) = 0$ for $r < R$. Analytically the energy eigenvalues of its Schrödinger equation can be calculated by matching the boundary conditions at radius $r = R$ [11]. Setting Planck constant $\hbar = 1$, the mass $m = 1$, and the pot radius $R = 2$, the exact energy eigenvalues for different potential height $V_0 = 20, 50$, and ∞ are denoted on the three bottom lines of Fig. 2. The dotted, dashed, and solid curves in the upper part

of Fig. 2 are the Fredholm determinant $|\det(1 - \mathcal{T}_m(E))|$ of the modified transfer operator for $V_0 = 20, 50$, and ∞ . The zeros of these functions determine the semiclassical quantum energies of the systems.

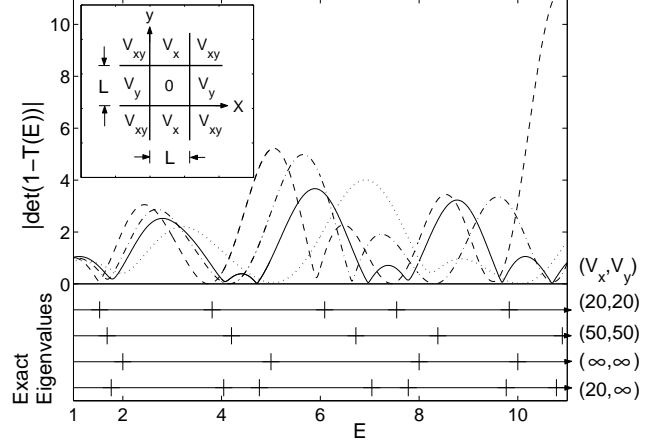


FIG. 3: The upper part shows the Fredholm determinant $|\det(1 - \mathcal{T}_m(E))|$ of the modified transfer operator $\mathcal{T}_m(E)$ for the square potential pot in the inset with the potential configuration $(V_x, V_y) = (20, 20), (50, 50), (20, \infty)$, and (∞, ∞) where $V_{xy} = V_x + V_y$. The points on the four bottom lines depict the exact quantum energies for $(V_x, V_y) = (20, 20), (50, 50), (20, \infty)$, and (∞, ∞) .

The second system is the 2D square quantum dot with the confining potential as shown in the inset of Fig. 3. Therein the xy -plane is separated into nine regions with different constant potential heights V_x, V_y , and V_{xy} at each region, where $V_x > 0, V_y > 0$, and $V_{xy} = V_x + V_y$. This 2D problem can be reduced to two independent 1D finite wells with potential heights V_x and V_y and solved separately [12]. Combining the eigenvalues of these two separated systems, the total quantum energies of this 2D system for $(V_x, V_y) = (20, 20), (50, 50), (20, \infty)$, and (∞, ∞) are determined and depicted on the four bottom lines in Fig. 3, where $\hbar = m = 1$ as before and the well length L is normalized by the condition $2\pi^2/L^2 = 1$. The upper part of this Figure shows the Fredholm determinants $|\det(1 - \mathcal{T}_m(E))|$ of the modified BTO. The dashed, dash-dotted, dotted, and solid curves represent these functions for the potential configurations $(V_x, V_y) = (20, 20), (50, 50), (\infty, \infty)$, and $(20, \infty)$.

Figure 2 and 3 shows surprisingly accurate quantum energies after the scattering phase correction. Taking Fig. 2 as example, the exact 10-th energy has a remarkable left shift after the potential height is reduced from $V_0 = \infty$ to $V_0 = 20$. This shows how large the error could be when simplifying a deep potential pot, even with the large ratio $V_0/R = 10$, by an infinitely high pot. Without scattering phase correction, the semiclassically calculated energies are the zeros of the solid curve. The 10-th zero of this curve is close to the 10-th point on the bottom

line of $V_0 = \infty$, but far apart from the 10-th point for $V_0 = 20$. However, after taking the scattering phase, the determinant (dotted curve) shifts leftward quite a lot and its zeros largely approach the exact energies for $V_0 = 20$.

Quantitatively we can define values to characterize these errors. Suppose E_i is the i -th exact energy of a quantum system bounded by some potential pot of height $V_0 < \infty$ and \tilde{E}_i is the corresponding semiclassical energy approximated by the modified BTO. Let the value $\delta_i = \tilde{E}_i - E_i$ be the difference between these two energies and the ratio $\Delta_i = \delta_i/E_i$ is the error of the i -th eigenvalue. For the special case of $V_0 = \infty$ the values defined above are furnished with a superscript ∞ as E_i^∞ , \tilde{E}_i^∞ , and $\delta_i^\infty = \tilde{E}_i^\infty - E_i^\infty$ respectively. The relative error Γ_i of the i -th energy is then defined as the ratio

$$\Gamma_i = \frac{|\delta_i - \delta_i^\infty|}{|E_i - E_i^\infty|}. \quad (9)$$

The denominator denotes the exact energy shift after the potential height is reduced from ∞ to V_0 . The numerator represents the error δ_i for $V_0 < \infty$ subtracted by the basic semiclassical error δ_i^∞ from infinite potential.

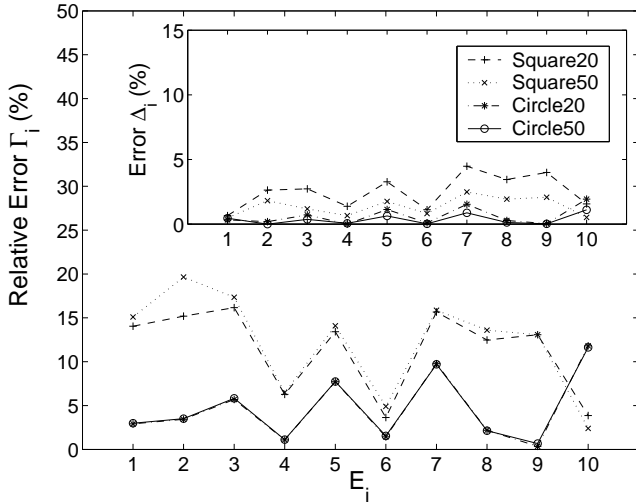


FIG. 4: The dotted and dashed curves in the main plot denote the relative errors Γ_i of the 2D circular potential pots with potential height 50 and 20, as shown in the inset of Fig. 2. The dash-dotted and solid curves represent Γ_i for the 2D square potential pots of configuration $(V_x, V_y) = (50, 50)$ and $(20, 20)$, as shown in the inset of Fig. 3. The corresponding errors δ_i of these systems are shown in the inset.

According to these definitions, the errors δ_i of the lowest ten energies from Fig. 2 and 3 are plotted in the inset of Fig. 4 and their corresponding relative errors Γ_i are plotted in its main figure. All δ_i are bounded by 5% and all Γ_i are bounded by 20%. Roughly speaking, the scattering phase in the modified BTO has corrected at least 80% of the energy error due to the potential reduction from ∞ to V_0 . This justifies the scattering phase correction proposed above for finitely confined systems.

Notably, one cannot expect 100% correction in this first order correction. Remember that there still exists other degrees of freedom in the system, which are not included in the scattering phase. For instance, the modified transfer operator $\mathcal{T}_m(E)$ is the same for square potential pots of different V_{xy} , although they have different quantum energies. This V_{xy} difference can only be distinguished from higher order corrections beyond the current scattering phase. Furthermore, if the particle energy E is close to the potential height V_0 , the particle can penetrate into the potential well quite long and the wave property of the particle prevails its particle property. In this regime, the correction deviation from the modified BTO increases. However, that is not because this first correction is wrong, but because higher order corrections are required in the semiclassical approach.

Finally, almost all semiclassical methods are based on the Green function of the quantum system. The successful result in the modified BOT gives a clear direction for extending the quantum correction to other semiclassical methods, including Gutzwiller trace formula, dynamical zeta functions, and Landauer-Büttiker formula.

We thank Hsiu-Hau Lin for fruitful discussions. This work was supported by the National Science Council at Taiwan under Grant Nos. NSC 93-2112-M-007-009.

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